

## **Electronic Supplementary Information**

### **Nanomolar level selective dual channel sensing of Cu<sup>2+</sup> and CN<sup>-</sup> from aqueous medium by an opto-electronic chemoreceptor**

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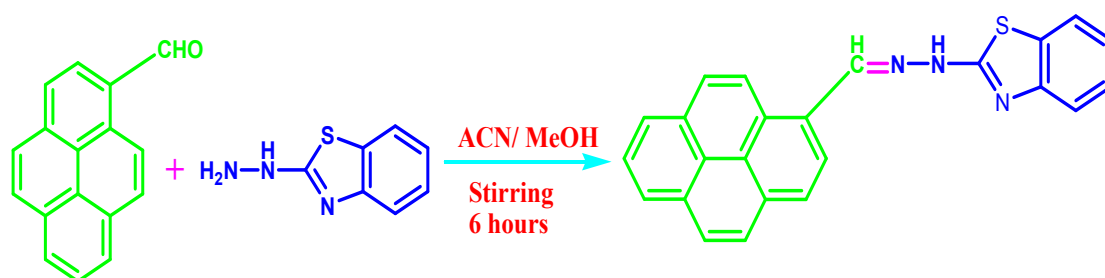
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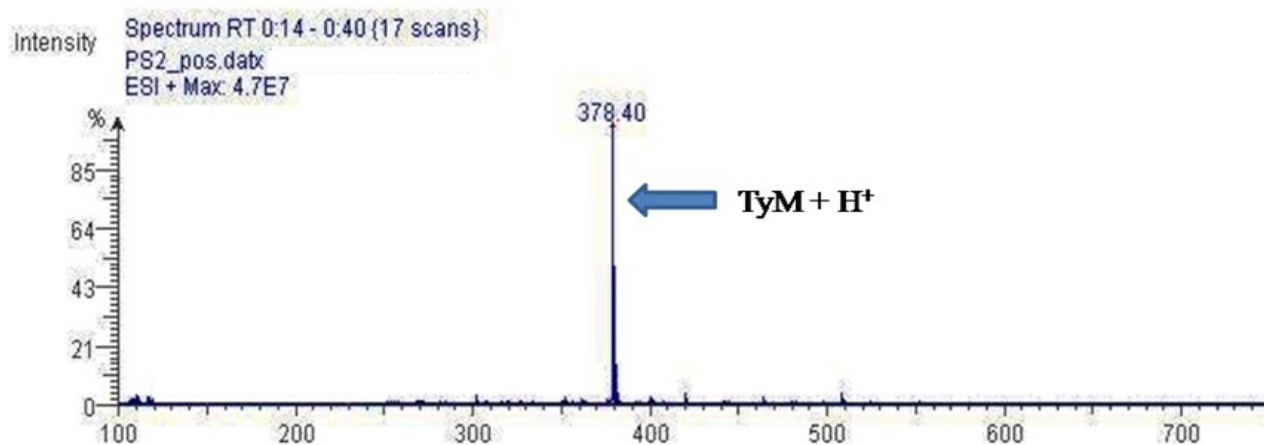
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## 1. Experimental

### Synthesis of TyM



**Scheme S1** Synthesis of chemoreceptor TyM.



**Fig. S1** ESI-MS of TyM in MeCN.

**Monoisotopic Mass, Odd and Even Electron Ions**

2 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 20-25 H: 12-17 N: 0-3 S: 0-1

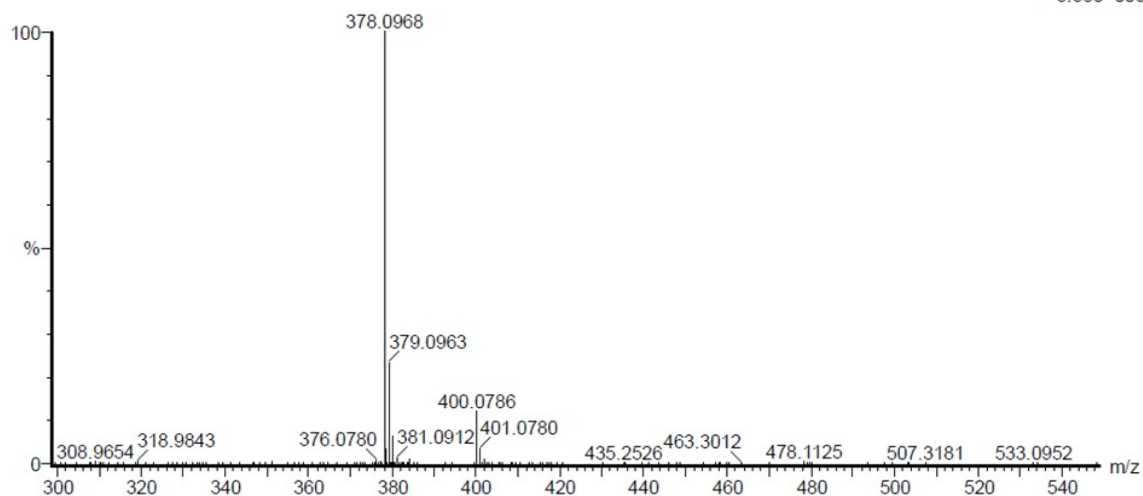
Sample Name : CMERI-01

Test Name : HRMS-1

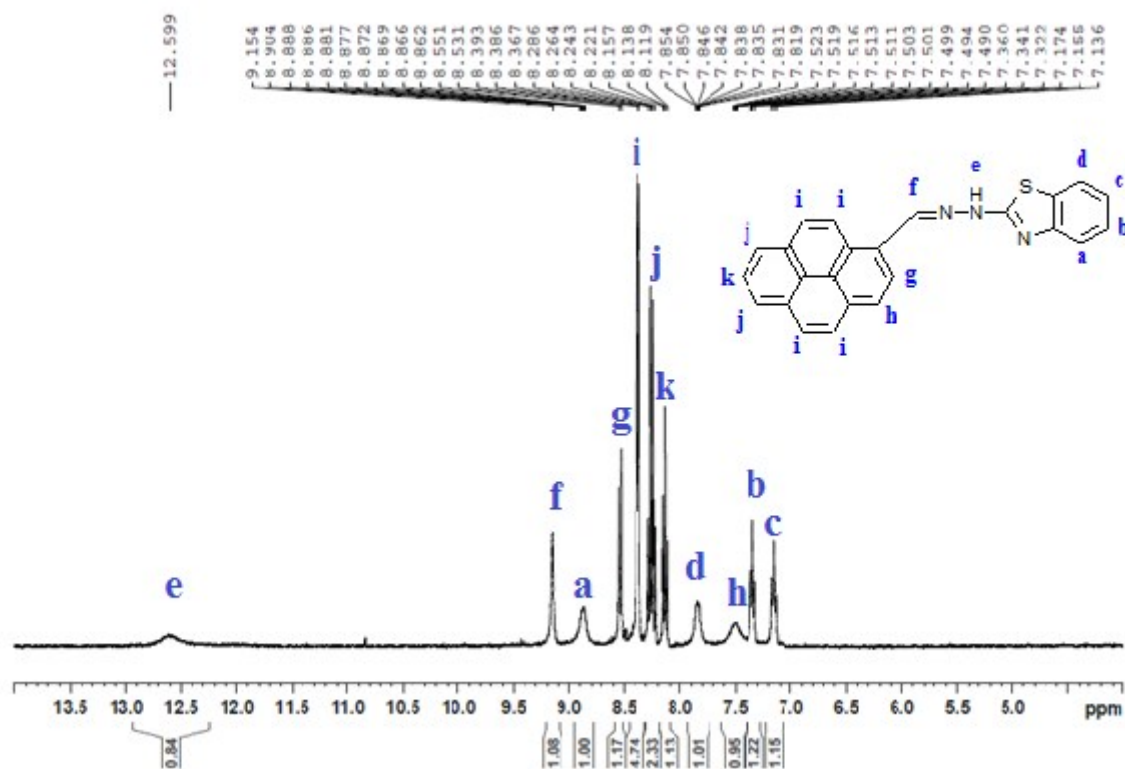
211117-CMERI-01 15 (0.168) AM (Top,4, Ar,10000.0,0.00,0.00); Cm (15:17-23:32)

XEVO G2-XS QTOF

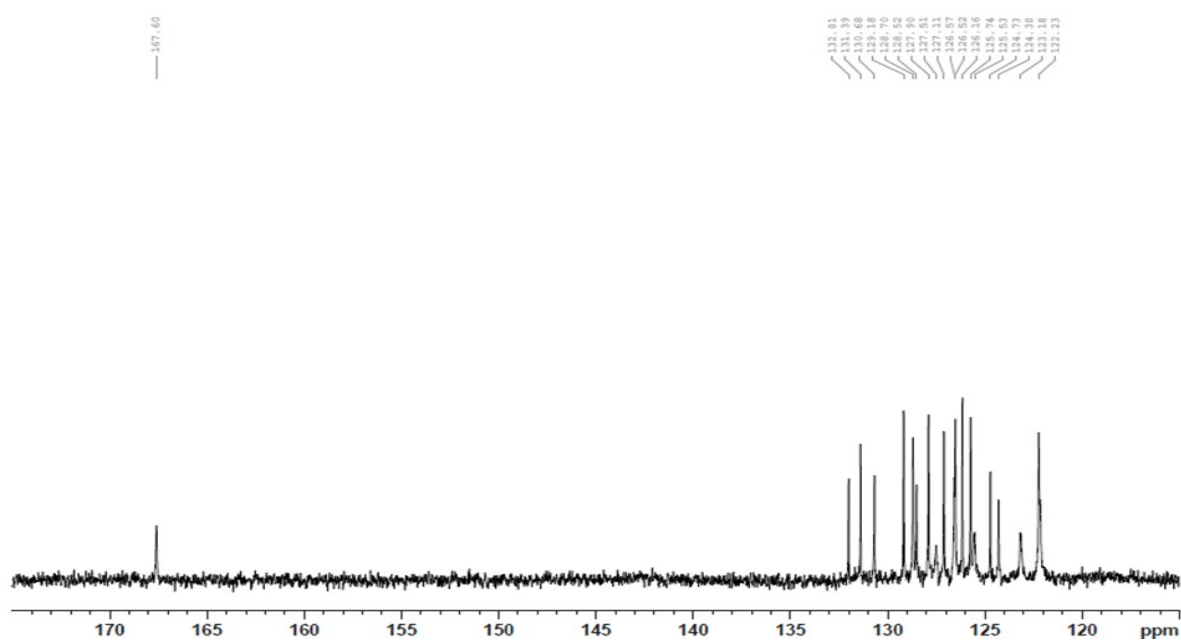
1: TOF MS ES+  
5.68e+006



**Fig. S2 HRMS of TyM in MeCN**



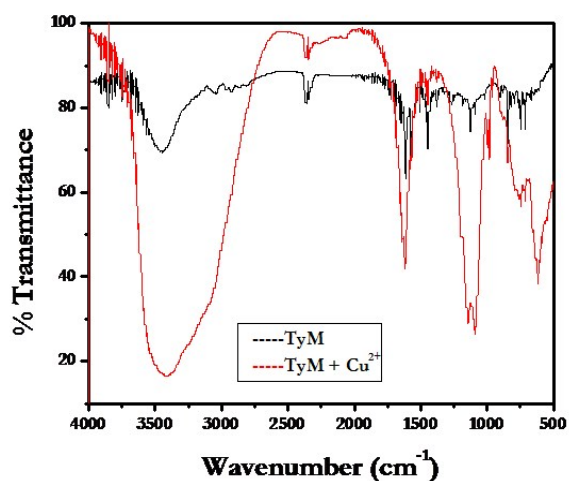
**Fig. S3**  $^1\text{H}$ -NMR of **TyM** in  $\text{DMSO-d}_6$ .



**Fig. S4**  $^{13}\text{C}$ -NMR of **TyM** in  $\text{DMSO-d}_6$

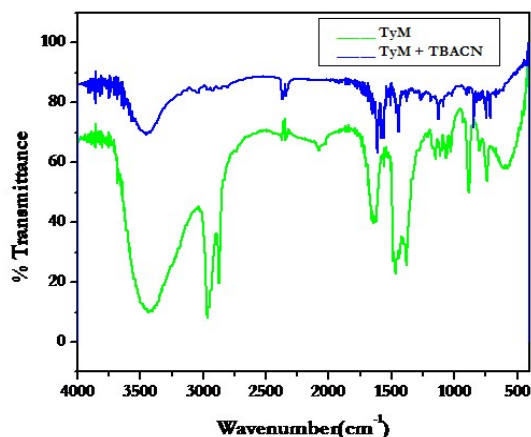
### IR Studies:

The FTIR spectrum of the chemoreceptor **TyM**, **TyM...Cu<sup>2+</sup>** and **TyM...CN<sup>-</sup>** complex were recorded in KBr disks. The existence of the peak at  $3440\text{ cm}^{-1}$  indicated the presence of secondary amine functional group in the chemoreceptor molecule. The peak at  $1630\text{ cm}^{-1}$  corresponds to the aldimine bond. This in turn affirms the formation of Schiff base between the aromatic aldehyde and hydrazine (herein 1-pyrene-carboxaldehyde and 2-hydrazino benzothiazole). When trace amount of  $\text{Cu}^{2+}$  was added to the chemoreceptor **TyM**, the peak at  $1630\text{ cm}^{-1}$  was shifted to a lower value of  $1600\text{ cm}^{-1}$  which confirms that the aldimine nitrogen atom present in the **TyM** molecule is involved in coordination with  $\text{Cu}^{2+}$ . On the contrary the lone pair of nitrogen in the  $-\text{NH}$  group present in the chemoreceptor molecule is getting delocalised after interaction with  $\text{CN}^-$  so the  $\text{N-H}$  bonded electron will be drifted towards nitrogen and therefore the  $-\text{NH}$  bond will be weak and broadened in nature.. This clearly suggests that  $\text{CN}^-$  interacts with  $\text{NH}$  proton of the secondary amine present in **TyM**. In addition there arises a new peak in the region of  $2800\text{ cm}^{-1}$  which corresponds to the formation of  $\text{H}\cdots\text{CN}^-$ .<sup>1</sup> The peaks from  $1600\text{ cm}^{-1}$  to



the region of  $1600\text{ cm}^{-1}$  to

500 cm<sup>-1</sup> also become flattened, which clearly implies an enhanced electronic distribution within the skeleton system with the addition of CN<sup>-</sup> ion (Fig. S5).



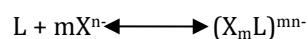
(a)

(b)

Fig. S5 FTIR spectra (a) TyM + Cu<sup>2+</sup> (b) TyM + CN<sup>-</sup>.

### Benesi-Hildebrand (B-H) Equation and Plot:

The association constant of a complex formed in between the chemoreceptor and the incoming targeted analytes has been determined from the following complex equilibrium.



$$K = \frac{[(X_mL)]^{mn-}}{[L][X^{n-}]^m}$$

For 1:1 type complex formation with m=1 the Benesi-Hildebrand relation is adopted which can be expressed in terms of optical density (A) as follows:

$$A = \frac{A_0 + A_1 K [X^{n-}]}{1 + K [X^{n-}]}$$

Or,

$$\frac{1}{A - A_0} = \frac{1}{(A_1 - A_0)} + \frac{1}{(A_1 - A_0) K [X^{n-}]}$$

Where [X<sup>n-</sup>], [L] and [(X<sub>m</sub>L)<sup>mn-</sup>] are the concentration of the added targeted analyte, chemoreceptor and complexation between the analyte and the chemoreceptor, respectively. A<sub>0</sub>, A and A<sub>1</sub> indicates the optical density or absorbance at a particular wavelength of **TyM** prior to the addition of the analyte, absorbance after adding the analyte at every successive step and finally excess amount of the added analyte, respectively. The binding constant or association constant K (M<sup>-1</sup>) is determined from the ratio of intercept and slope of Benesi-Hildebrand plot of optical density. As depicted in the following In the Benesi-Hildebrand (B-H) plot of 1/[A-A<sub>0</sub>] vs 1/[CN<sup>-</sup>] for the titration of the chemoreceptor **TyM** and CN<sup>-</sup> provides a straight line (best fitted), indicating a 1:1 type complex formation with association constant K = 0.98 x 10<sup>6</sup> M<sup>-1</sup> (Fig. S6)

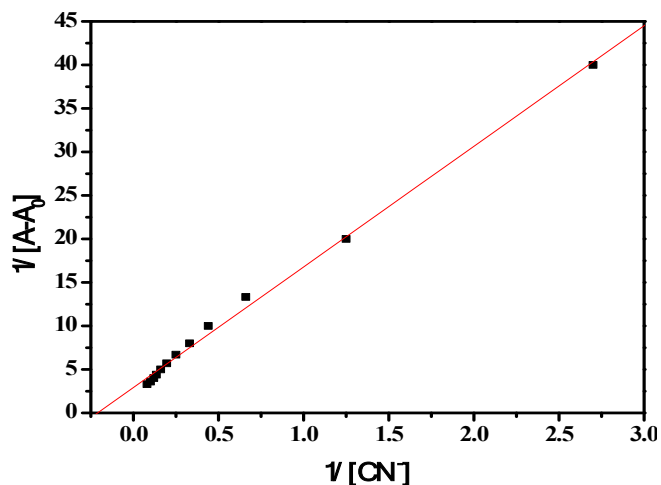


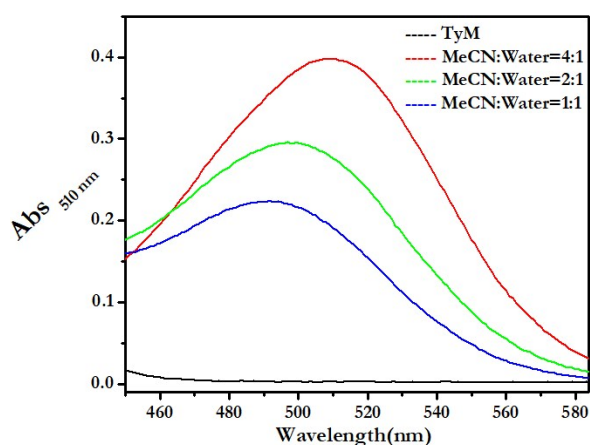
Fig. S6 B-H plot of chemoreceptor **TyM** vs.  $\text{CN}^-$ .

### Colorimetric response and Optical performance:

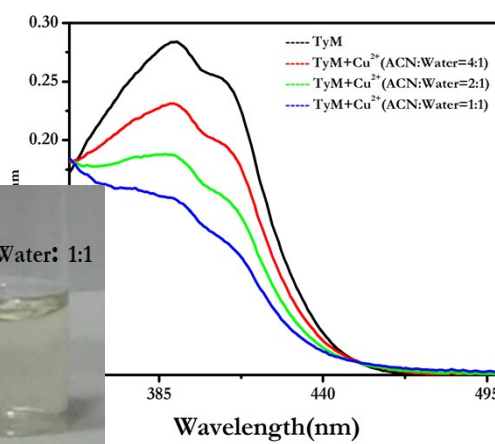
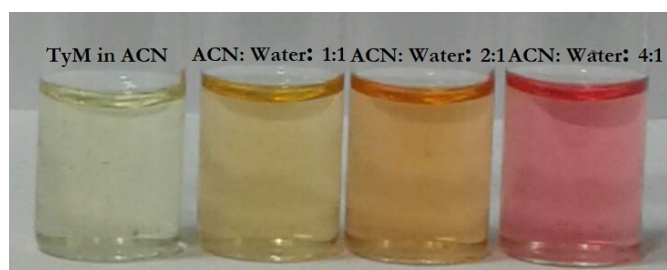
The colorimetric response and optic performances of the chemoreceptor has been investigated in presence of varying solvent mixture.

The UV-Vis study of the chemoreceptor in presence of targeted analyte (*i.e.*;  $\text{Cu}^{2+}$  and  $\text{CN}^-$ ) in varying solvent mixture has been carried out. In case of  $\text{CN}^-$  the absorbance at 510 nm has been monitored carefully. The figure indicates that the sensing is possible even in presence of water which undoubtedly establishes the superiority of the chemoreceptor. In semi aqueous medium [ACN:Water (4:1, v/v)] the detection shows red coloration owing to the strong adduct formation which is also noticed in case of ACN:Water (1:1, v/v) solvent mixture. Indeed the affinity of the developed chemoreceptor towards  $\text{CN}^-$  is established.

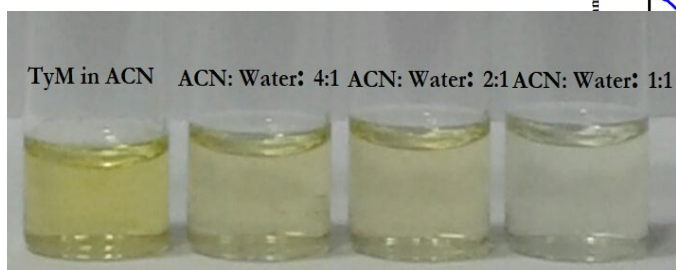
The detection of  $\text{Cu}^{2+}$  reported herein no way encounters any interference from the existence of water since the chemoreceptor designed exhibits its proclivity towards  $\text{Cu}^{2+}$  and the luminescence is although enhanced in presence of water however the individual detection occurs at completely different spectroscopic energy levels clearly stating that the detection of  $\text{Cu}^{2+}$  is not a consequence of existence of aqueous medium in the sample.



(a)



(b)

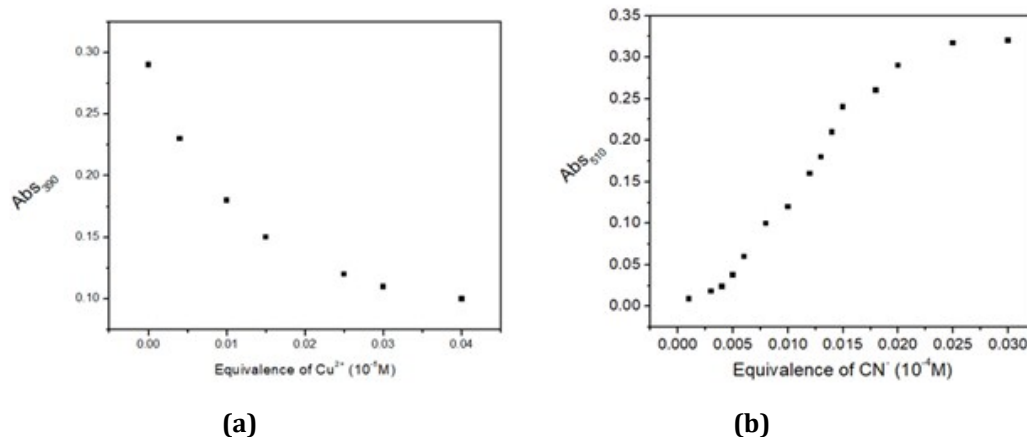


(c)

(d)

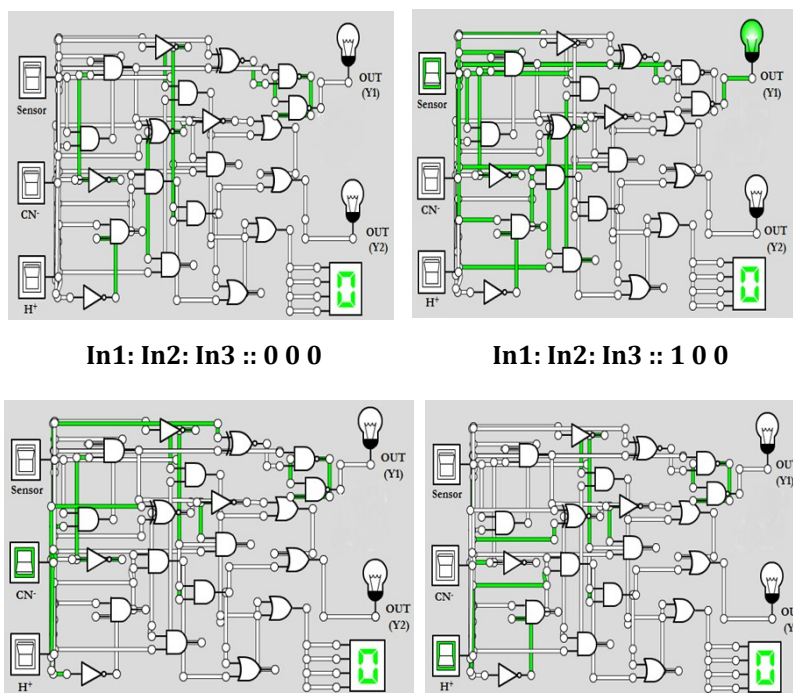
**Fig. S7** (a) UV-Vis absorption changes of **TyM** with gradual addition of  $\text{CN}^-$  ( $1 \times 10^{-4}\text{M}$ ) in varying proportion of  $\text{CH}_3\text{CN}$  and  $\text{H}_2\text{O}$ . (b) Colorimetric changes of **TyM** with  $\text{CN}^-$  in varying proportion of  $\text{CH}_3\text{CN}$  and  $\text{H}_2\text{O}$ . (c) UV-Vis absorption changes of **TyM** with gradual addition of  $\text{Cu}^{2+}$  ( $1 \times 10^{-4}\text{M}$ ) in varying proportion of  $\text{CH}_3\text{CN}$  and  $\text{H}_2\text{O}$ . (d) Colorimetric changes of **TyM** with  $\text{Cu}^{2+}$  in varying proportion of  $\text{CH}_3\text{CN}$  and  $\text{H}_2\text{O}$ .

The linearity range of colorimetric response of  $\text{Cu}^{2+}$  and  $\text{CN}^-$  is plotted and placed hereby:

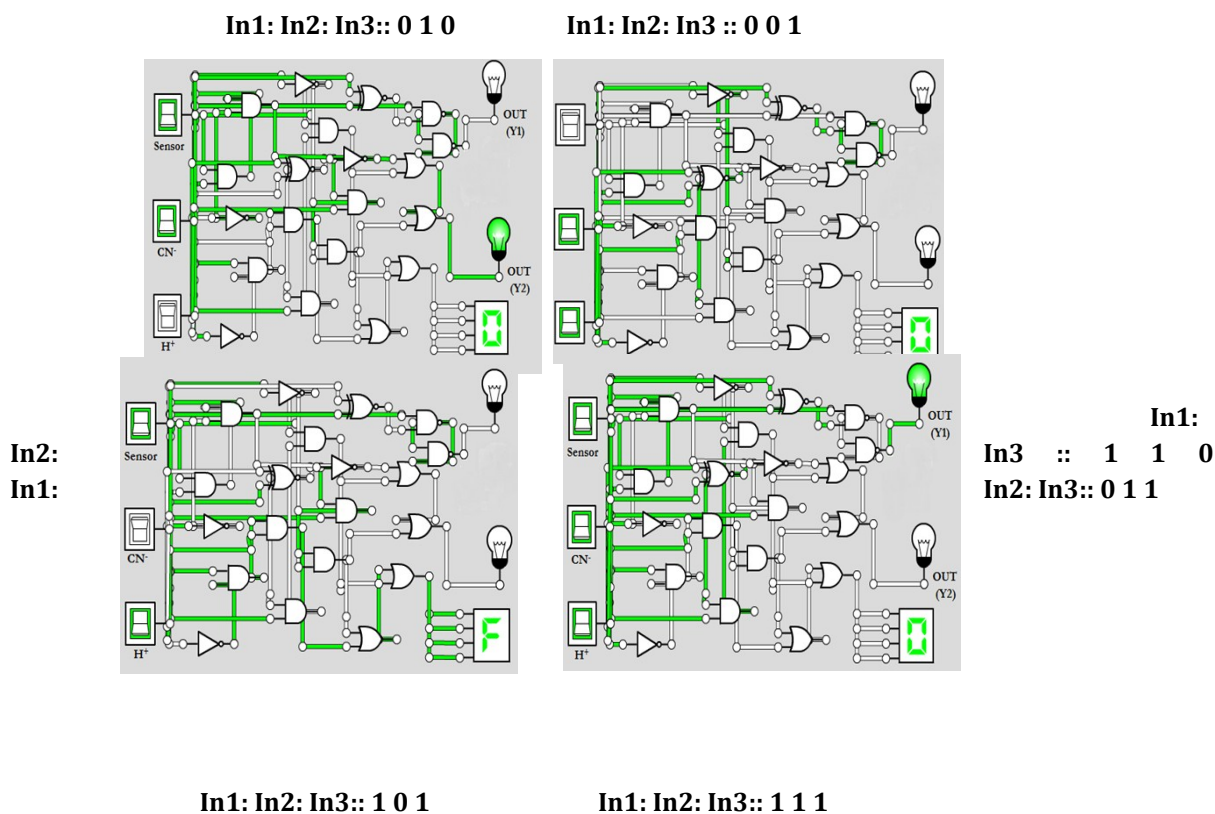


**Fig. S8** Linearity range of colorimetric response of **TyM** towards (a)  $\text{Cu}^{2+}$ , (b)  $\text{CN}^-$ .

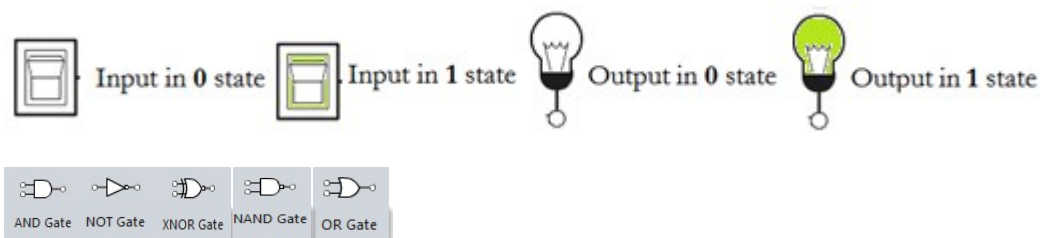
**Electronic circuit fabrication based on different logic gates:**







**Fig. S9** Fabrication of logic gate with outputs (Y1 and Y2) upon varying inputs AND-NOT-XNOR-NAND-OR logic functions.

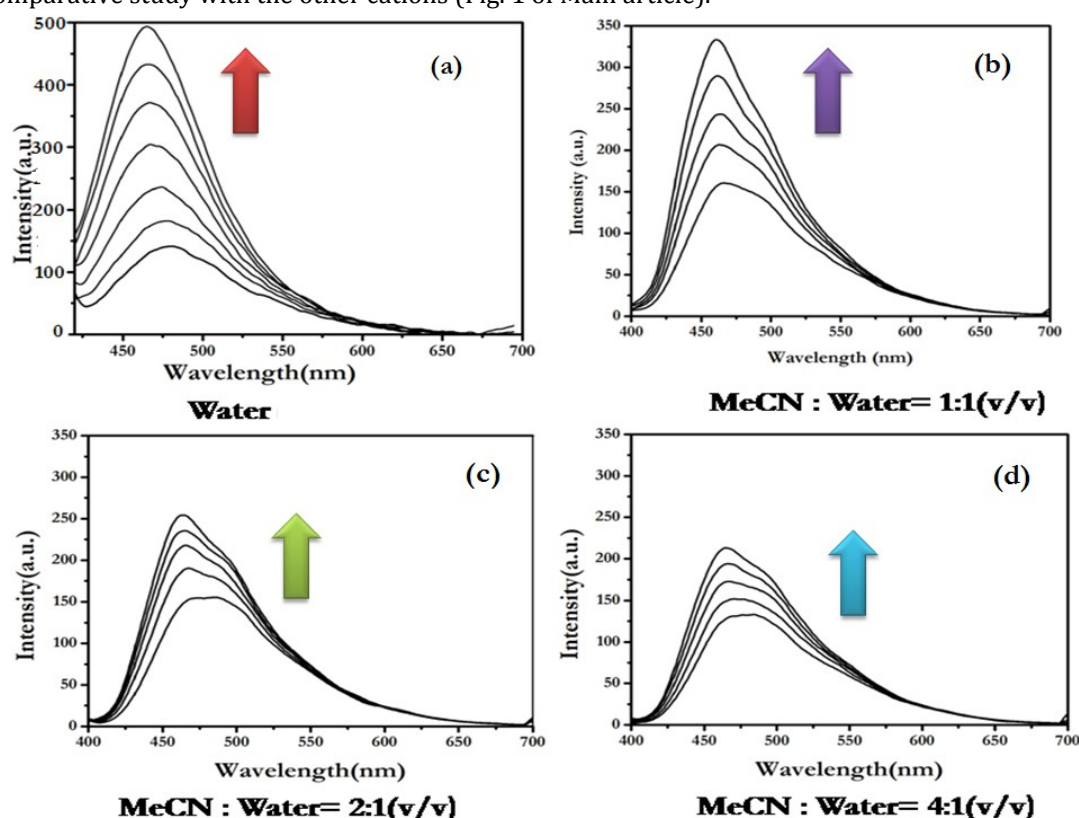


### Effect of Water:

Upon gradual addition of water to the acetonitrile solution of chemoreceptor **TyM** the luminescence of the bare chemoreceptor **TyM** was enhanced with the simultaneous shift in the emission profile. The initial peak at 485 nm was shifted to 460 nm after addition of water. Pyrene moiety being an aromatic fused hydrophobic ring when encounters water molecules in its surrounding it tends to form an aggregate which consequences in enhancement of the photoluminescence property of the chemoreceptor **TyM** via Aggregation Induced Emission Enhancement (AIEE). The effect of water has not been interfering during the detection of  $\text{Cu}^{2+}$  in the aqueous medium since the response of the chemoreceptor **TyM** towards water as well as  $\text{Cu}^{2+}$  was at completely different spectroscopic energy. In case of water the fluorescence of the solution was feebly enhanced along with change in spectroscopic wavelength from 485 nm to 460 nm during the increase in the luminescence. On the contrary  $\text{Cu}^{2+}$  leads to a manifold enhancement in emission accompanied by a transition in luminescence from green to cyan.



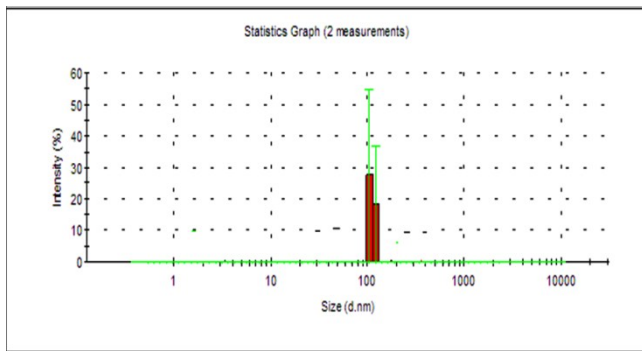
From the figure it is quite evident that with increase in percentage of water the emission intensity of the chemoreceptor **TyM** has increased. The trend in the increase of emission intensity follows the order; Water > ACN:Water (1:1, v/v) > ACN:Water (2:1, v/v) > ACN:Water (4:1, v/v) (Fig. S10). The outcome of the fluorometric response is a direct consequence of the varying proportion of water. It is ascertained that with the increase in water exhibit a driving force in alleviation of luminescence of the probe. Herein the peak at 485 nm corresponding to the inherent fluorescence of the chemoreceptor has been shifted to 460 nm after addition of water. Owing to the fact that the fluorophore pyrene moiety being an aromatic fused hydrophobic ring when encounters water molecules in its surrounding it tends to form an aggregate. Furthermore this aggregation consequence in enhancement of photoluminescence property of the chemoreceptor **TyM** via aggregation induced emission enhancement (AIEE)<sup>2</sup>. However the addition of water to the chemoreceptor solution doesn't induce any colorimetric change which is also evident from the comparative study with the other cations (Fig. 1 of Main article).



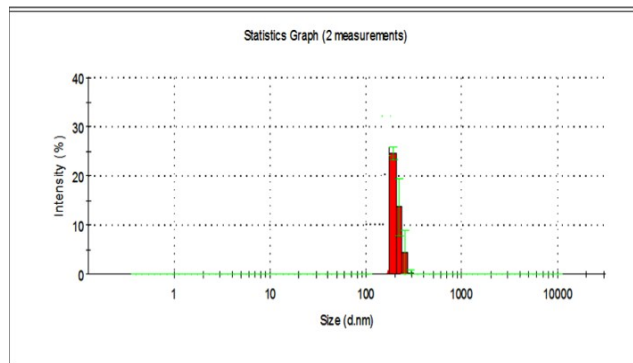
**Fig. S10** Fluorescence spectra of TyM in varying proportion of CH<sub>3</sub>CN and H<sub>2</sub>O. **(a)** Water, **(b)** MeCN : Water = 1:1(v/v), **(c)** MeCN : Water = 2:1 (v/v), **(d)** MeCN : Water = 4:1(v/v)

#### Evidence in favour of AIEE:

Dynamic light scattering (DLS) is a technique that can be used to determine the size distribution profile of small particles in suspension or polymers in solution. If the system is mono dispersed, there should only be one population, whereas a poly dispersed system would show multiple particle populations. DLS has been executed herein in order to assess the particle size of the sole chemoreceptor **TyM** and the variation in its dimension after interaction with the water. The outcome is in line with the speculation. The initial size of **TyM** is ~ 110nm whereas a substantial enhancement in the size has been observed (~ 340nm) after interaction with water due to the agglomeration of the **TyM** particles in the aqueous environment. Formation of aggregate of the chemoreceptor molecule in existence of water is truly reflected in its emission properties thus satisfying Aggregation Induced Emission Enhancement (AIEE) phenomenon.



(a)



(b)

**Fig. S11** Particle size determination of (a) **TyM** (b) **TyM** + H<sub>2</sub>O.

The association constant for 2:1 complexation of **TyM** : Cu<sup>2+</sup> has been determined by employing equation 1:

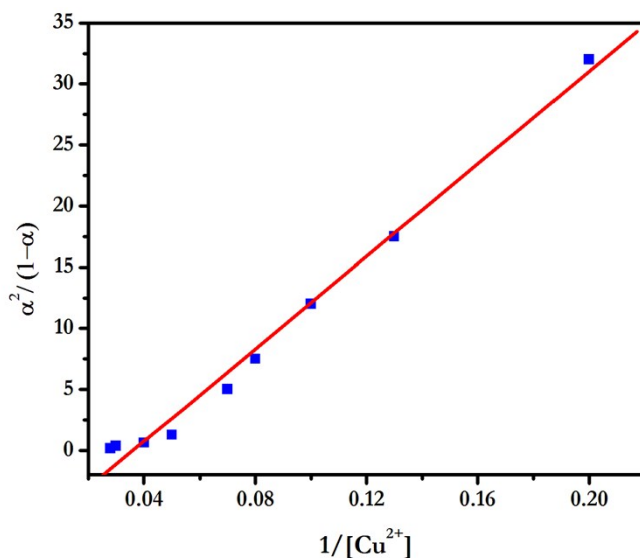
$$\frac{\alpha^2}{1 - \alpha} = \frac{1}{2K_a C_F [M]} \dots\dots\dots (1)$$

where, C<sub>F</sub> is the total concentration of **TyM** in the system and “α” is defined as the ratio between the free chemoreceptor **TyM** and its total concentration. The value “α” has been obtained using equation 2:

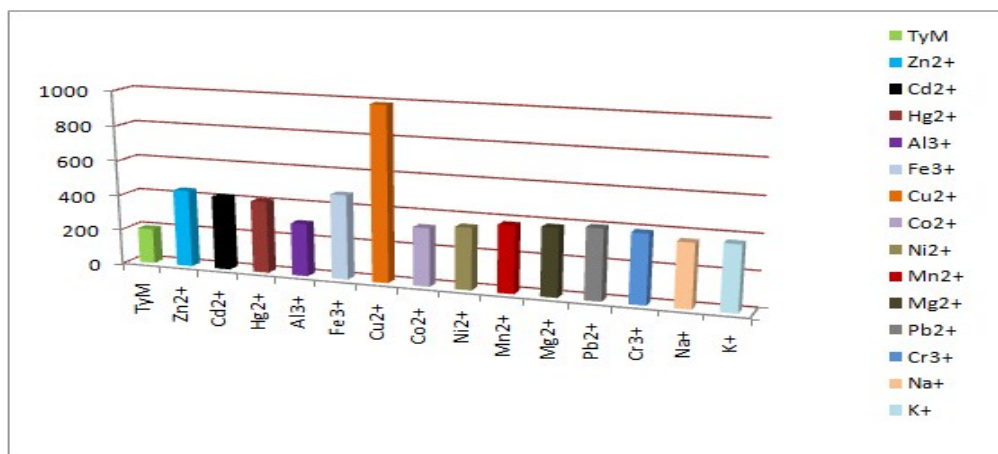
$$\alpha = \frac{F - F_0}{F_1 - F_0} \dots\dots\dots (2)$$

where F is the fluorescence intensity at 485 nm at any given concentration of the analyte (Cu<sup>2+</sup> herein), F<sub>1</sub> is the fluorescence intensity at 485 nm in the absence of Cu<sup>2+</sup>, F<sub>0</sub> is the maxima fluorescence intensity at 485 nm in the presence of Cu<sup>2+</sup>. The association constant K<sub>a</sub> has been evaluated graphically by plotting  $\frac{\alpha^2}{1 - \alpha}$

against 1/[Cu<sup>2+</sup>] and is shown in Fig. S12. The data so obtained has been linearly fitted according to Eq. (1) and the K<sub>a</sub> value has been obtained from the slope of the line. The association constant has been evaluated to be 0.1 x 10<sup>5</sup> M<sup>-2</sup>.

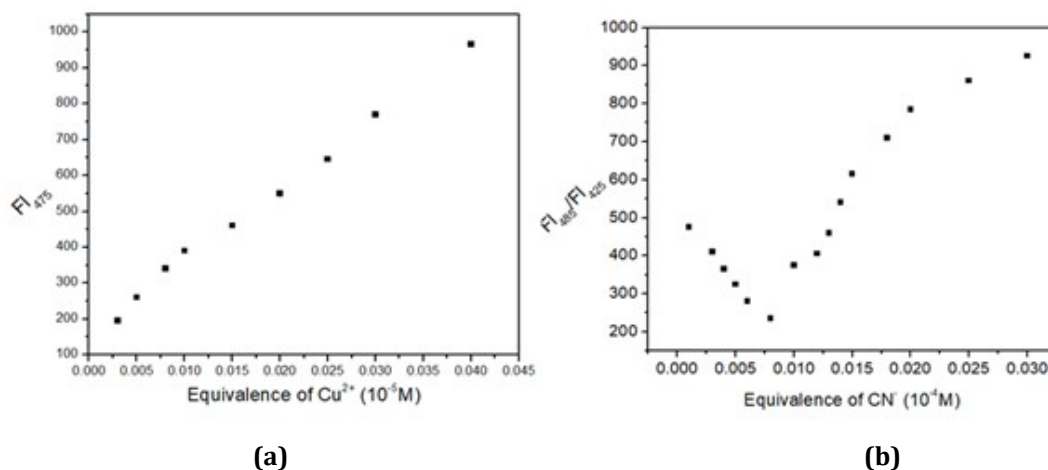


**Fig. S12** Association constant determination of chemoreceptor **TyM** vs.  $\text{Cu}^{2+}$ .



**Fig. S13** Comparative study of the chemoreceptor **TyM** in presence of other cations.

The linearity range of fluorometric response of  $\text{Cu}^{2+}$  and  $\text{CN}^-$  is plotted and placed hereby:



**Fig. S14** Linearity range of fluorescent detection of **TyM** towards **(a)**  $\text{Cu}^{2+}$ , **(b)**  $\text{CN}^-$ .

**Table S1** – Geometry optimized coordinates of **TyM**.

|   |             |             |              |
|---|-------------|-------------|--------------|
| N | 4.449344600 | 5.760345501 | 9.688249293  |
| N | 4.682333133 | 5.143017679 | 10.910655213 |
| C | 4.991362570 | 6.237767416 | 4.870920921  |
| C | 5.324802965 | 5.677587759 | 3.615524187  |
| C | 4.467962577 | 7.549194695 | 4.925886734  |
| C | 5.176332801 | 5.486864911 | 6.063693211  |
| C | 4.123560237 | 8.104879419 | 6.160106414  |
| C | 5.832645874 | 4.363256289 | 3.540683343  |

|   |             |             |              |
|---|-------------|-------------|--------------|
| C | 5.146254788 | 6.430945989 | 2.431543286  |
| C | 4.843378983 | 6.078248854 | 7.315905950  |
| C | 5.078011407 | 5.387877626 | 8.614569021  |
| C | 4.307901209 | 7.380632628 | 7.335895626  |
| C | 4.293401592 | 8.285476174 | 3.744041266  |
| C | 5.665578442 | 4.165531148 | 5.955084524  |
| C | 4.632160546 | 7.732063191 | 2.507451598  |
| C | 5.993711072 | 3.617699767 | 4.712602267  |
| C | 6.161640320 | 3.814636005 | 2.291719874  |
| C | 5.482395151 | 5.866304015 | 1.192080565  |
| C | 5.987546475 | 4.565186380 | 1.125875412  |
| C | 2.539044516 | 8.370211798 | 14.428124730 |
| C | 2.914444266 | 7.427279379 | 13.474385552 |
| C | 1.994342283 | 6.570433245 | 12.886438014 |
| C | 0.646156082 | 6.631149840 | 13.243378896 |
| C | 0.243359338 | 7.572763919 | 14.205927367 |
| C | 1.185721459 | 8.438840509 | 14.795148914 |
| S | 4.457359677 | 7.122960223 | 12.844448511 |
| C | 3.861808602 | 5.878097652 | 11.840890307 |
| N | 2.509729662 | 5.701592351 | 11.962786617 |
| H | 4.143097800 | 4.227643740 | 10.819095037 |
| H | 3.717009057 | 9.111151990 | 6.219098180  |
| H | 5.804184273 | 4.582235688 | 8.689792836  |
| H | 4.048644195 | 7.858842094 | 8.276263835  |
| H | 3.892278471 | 9.295097457 | 3.776498301  |
| H | 5.786285289 | 3.525023215 | 6.818651978  |
| H | 4.487542933 | 8.322562526 | 1.606555395  |
| H | 6.371054414 | 2.599338326 | 4.668705700  |
| H | 6.552550587 | 2.803404449 | 2.216457870  |
| H | 5.352692284 | 6.431233247 | 0.272945962  |
| H | 6.243768087 | 4.134317375 | 0.163011652  |
| H | 3.271751933 | 9.033799053 | 14.876204126 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| H | -0.079066765 | 5.963729886 | 12.788305577 |
| H | -0.800561893 | 7.632995177 | 14.497155102 |
| H | 0.864008507  | 9.162753294 | 15.536989457 |

**Table S2** – Geometry optimized coordinates of **TyM•••CN<sup>-</sup>**.

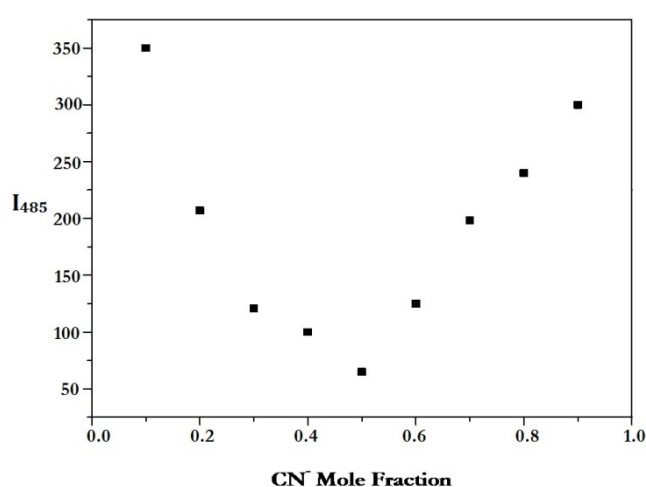
|   |             |             |              |
|---|-------------|-------------|--------------|
| N | 4.505661725 | 6.711771097 | 9.847287874  |
| N | 5.017432647 | 6.936733467 | 11.104594350 |
| C | 4.805580796 | 5.770387575 | 5.093193677  |
| C | 5.523605093 | 5.216976250 | 4.007853739  |
| C | 3.479751031 | 6.215895153 | 4.891520597  |
| C | 5.410408978 | 5.872594296 | 6.374566549  |
| C | 2.758081668 | 6.747018650 | 5.963476059  |
| C | 6.841257229 | 4.748712361 | 4.197829113  |
| C | 4.921936047 | 5.127165047 | 2.730805058  |
| C | 4.670925192 | 6.443104183 | 7.447466078  |
| C | 5.262804744 | 6.662374185 | 8.793184140  |
| C | 3.344232300 | 6.855969493 | 7.222957452  |
| C | 2.893333634 | 6.119655401 | 3.620416244  |
| C | 6.722259456 | 5.375829699 | 6.540898039  |
| C | 3.609509202 | 5.582933529 | 2.548196441  |
| C | 7.426406428 | 4.827808443 | 5.465873263  |
| C | 7.546994340 | 4.200811589 | 3.115898107  |
| C | 5.644342979 | 4.579054895 | 1.660333734  |
| C | 6.949657732 | 4.119512360 | 1.855052849  |
| C | 1.296491305 | 6.505275273 | 14.638129914 |
| C | 2.420614979 | 6.676605447 | 13.834299152 |
| C | 3.658157210 | 7.014755664 | 14.363985860 |
| C | 3.808011483 | 7.206156352 | 15.738346994 |
| C | 2.687286152 | 7.041209973 | 16.570057471 |
| C | 1.437707910 | 6.689224011 | 16.022569965 |
| S | 2.545961766 | 6.516587595 | 12.152862749 |
| C | 4.215332892 | 6.891975238 | 12.189379147 |
| N | 4.673142077 | 7.135283693 | 13.453550522 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| N | 3.973980885 | 3.449027433 | 9.994173149  |
| C | 5.379607248 | 3.333564823 | 10.273984036 |
| N | 4.536023299 | 2.697173152 | 14.968487393 |
| C | 4.671676601 | 3.754202329 | 16.009091673 |
| C | 3.919676048 | 3.281216298 | 13.744710865 |
| C | 5.882246220 | 2.153303073 | 14.634816658 |
| C | 3.670608075 | 1.600247732 | 15.485347923 |
| H | 6.038788851 | 7.149663811 | 11.234184241 |
| H | 1.736193393 | 7.090610040 | 5.825677351  |
| H | 6.336479623 | 6.799803453 | 8.902588395  |
| H | 2.758821181 | 7.295965704 | 8.025510076  |
| H | 1.874939988 | 6.461304768 | 3.454927362  |
| H | 7.218469607 | 5.382735701 | 7.503234273  |
| H | 3.133269317 | 5.519811971 | 1.573410121  |
| H | 8.435096758 | 4.457779821 | 5.630153214  |
| H | 8.561854941 | 3.834297973 | 3.245342846  |
| H | 5.198317232 | 4.503726856 | 0.672209586  |
| H | 7.502004563 | 3.694828969 | 1.022625405  |
| H | 0.337574251 | 6.235512989 | 14.207227134 |
| H | 4.772646071 | 7.471632982 | 16.159633588 |
| H | 2.786262619 | 7.182119138 | 17.641583657 |
| H | 0.579483013 | 6.559942614 | 16.674344928 |
| H | 5.319205508 | 4.587784192 | 15.647055375 |
| H | 5.129653759 | 3.341403502 | 16.939258495 |
| H | 3.675167696 | 4.179350174 | 16.275996154 |
| H | 2.911213387 | 3.702715311 | 13.968899977 |
| H | 3.800262844 | 2.506635529 | 12.950504090 |
| H | 4.554233911 | 4.101080000 | 13.332844966 |
| H | 5.808407310 | 1.357524681 | 13.855847594 |
| H | 6.367074265 | 1.709279454 | 15.536698357 |
| H | 6.550854918 | 2.957189869 | 14.244326142 |
| H | 2.654892002 | 1.983249800 | 15.744828906 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| H | 4.112075123 | 1.143451208 | 16.403038895 |
| H | 3.551102769 | 0.794297912 | 14.722654470 |

### Jobs Plot Analysis of TyM with CN<sup>-</sup>:

The stoichiometric ratio of the chemoreceptor **TyM** with CN<sup>-</sup> successive solutions comprising of 10<sup>-4</sup> M NBu<sub>4</sub>CN and **TyM** were prepared in acetonitrile solvent in such a way that the total concentration of the resulting solution remains constant. The mole fraction of the added analyte CN<sup>-</sup> was varied from 0.1 to 0.9. The emission of the chemoreceptor **TyM** at 485 nm has been plotted against the mole fraction of the added analyte. From the Jobs Plot analysis it clearly affirms a 1:1 complexation between the host chemoreceptor **TyM** and the guest analyte (Fig. S15).



**Fig. S15** Job's plot of chemoreceptor **TyM** with CN<sup>-</sup> with a total concentration of 10<sup>-4</sup> M.

**Table S3** – Geometry optimized coordinates of **TyM**•••Cu<sup>2+</sup> (1:1).

|   |             |             |              |
|---|-------------|-------------|--------------|
| N | 4.419052915 | 6.200593960 | 9.518213073  |
| N | 4.678603462 | 5.756452358 | 10.794408681 |
| C | 4.971261911 | 6.232795713 | 4.687927959  |
| C | 5.361674832 | 5.568618460 | 3.501740668  |
| C | 4.306442590 | 7.476513411 | 4.597821255  |
| C | 5.238721483 | 5.651129663 | 5.956730954  |
| C | 3.904288304 | 8.131767205 | 5.764014069  |
| C | 6.010577355 | 4.317633728 | 3.573225414  |
| C | 5.098128200 | 6.153277171 | 2.240851311  |
| C | 4.839763545 | 6.342390462 | 7.135630997  |
| C | 5.136939403 | 5.829833938 | 8.500800493  |



|    |              |             |              |
|----|--------------|-------------|--------------|
| C  | 4.166104267  | 7.572598746 | 7.013016051  |
| C  | 4.049684896  | 8.045454320 | 3.341106695  |
| C  | 5.870613992  | 4.387881172 | 5.996375367  |
| C  | 4.444333001  | 7.390602397 | 2.172498682  |
| C  | 6.254890573  | 3.736798351 | 4.821644608  |
| C  | 6.394893562  | 3.665031892 | 2.392001226  |
| C  | 5.490919120  | 5.486414084 | 1.070684711  |
| C  | 6.136356472  | 4.249515531 | 1.149257989  |
| C  | 2.192235869  | 6.696116586 | 15.350792170 |
| C  | 2.706759927  | 6.560640768 | 14.128136853 |
| C  | 2.118904664  | 7.204624968 | 12.959770222 |
| C  | 1.025596299  | 7.963912123 | 13.079956044 |
| C  | 0.425673039  | 8.136662492 | 14.429353660 |
| C  | 0.977975815  | 7.536873689 | 15.503795001 |
| S  | 4.134648603  | 5.631259401 | 13.592851757 |
| C  | 3.848997904  | 6.160140639 | 11.880179502 |
| N  | 2.806599186  | 6.942822037 | 11.716667918 |
| Cu | 1.070191904  | 7.689836571 | 8.880458017  |
| H  | 5.487521391  | 5.114021484 | 10.986789795 |
| H  | 3.389937017  | 9.087871810 | 5.711451488  |
| H  | 5.972792292  | 5.153353538 | 8.662760977  |
| H  | 3.856075046  | 8.124161177 | 7.896041151  |
| H  | 3.540029215  | 9.002098854 | 3.261781604  |
| H  | 6.062292780  | 3.871528445 | 6.927908830  |
| H  | 4.233850832  | 7.852022695 | 1.211359492  |
| H  | 6.740808818  | 2.766992673 | 4.891266992  |
| H  | 6.894724134  | 2.700811129 | 2.429507490  |
| H  | 5.297045815  | 5.921281941 | 0.093826968  |
| H  | 6.436544369  | 3.738669286 | 0.239671410  |
| H  | 2.645559006  | 6.206186288 | 16.206272460 |
| H  | 0.582778760  | 8.443519912 | 12.212807350 |
| H  | -0.462708496 | 8.749107085 | 14.546981167 |

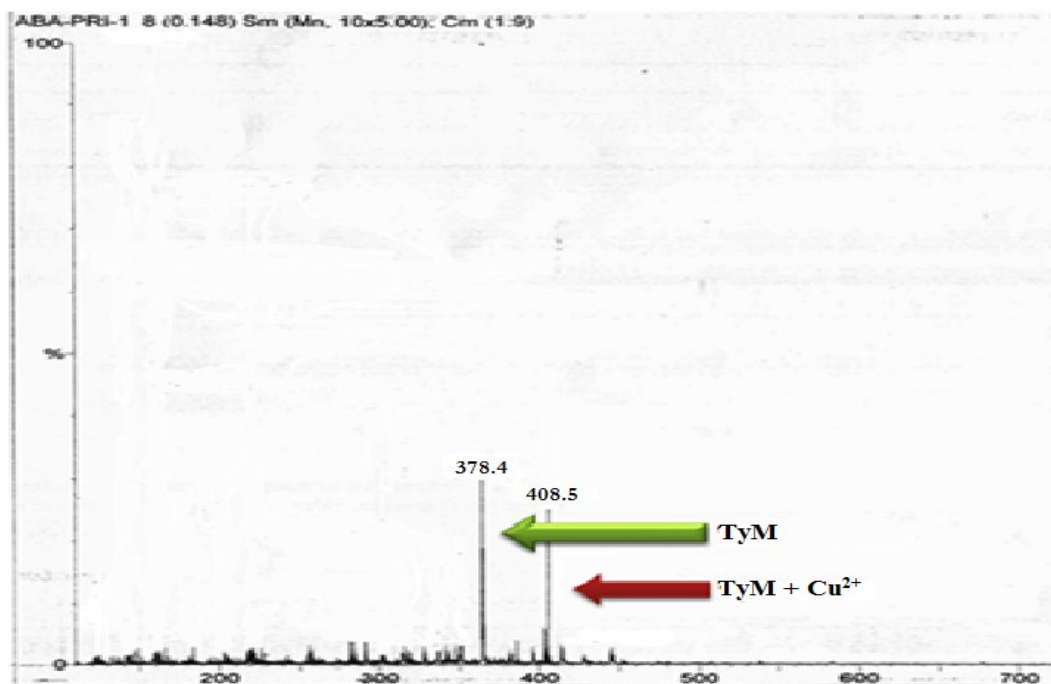
H 0.534534503 7.666470052 16.485894163

**Table S4** – Geometry optimized coordinates of **TyM•••Cu<sup>2+</sup>** (2:1).

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | 2.423819563  | 8.612024123  | 11.613226542 |
| N | 1.646418895  | 8.339705806  | 12.726535839 |
| C | 3.488372337  | 7.745302739  | 6.996552230  |
| C | 3.112737027  | 7.085338312  | 5.804058750  |
| C | 4.437393079  | 8.790876368  | 6.942618847  |
| C | 2.907053096  | 7.369018766  | 8.235258864  |
| C | 4.822204049  | 9.437098659  | 8.121122311  |
| C | 2.158870776  | 6.045882558  | 5.841762282  |
| C | 3.682400447  | 7.473337263  | 4.569410042  |
| C | 3.305169464  | 8.044082894  | 9.421423169  |
| C | 2.737793869  | 7.696571755  | 10.745496356 |
| C | 4.272536511  | 9.056714487  | 9.344020392  |
| C | 4.990781719  | 9.170626522  | 5.710654239  |
| C | 1.927323396  | 6.351035108  | 8.238109795  |
| C | 4.615957273  | 8.517885743  | 4.533739104  |
| C | 1.569310561  | 5.693250873  | 7.059568168  |
| C | 1.796066980  | 5.391955470  | 4.655103820  |
| C | 3.301678556  | 6.812639091  | 3.391895362  |
| C | 2.366654997  | 5.775083976  | 3.438437941  |
| C | -0.736548598 | 11.800446087 | 15.758984236 |
| C | -0.020451725 | 11.020759297 | 14.854082762 |
| C | 0.761263896  | 11.596002321 | 13.857970358 |
| C | 0.861297412  | 12.980762740 | 13.734987709 |
| C | 0.146782000  | 13.785267747 | 14.639346649 |
| C | -0.648974554 | 13.198216446 | 15.645000038 |
| S | 0.069893740  | 9.315181912  | 14.755002150 |
| C | 1.124389717  | 9.398087132  | 13.416026749 |
| N | 1.387805441  | 10.689425438 | 13.058103819 |
| N | 2.449132341  | 11.710743421 | 9.935982877  |
| N | 3.509880159  | 12.600465376 | 9.968594668  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | -0.449118634 | 8.780914434  | 7.432611665  |
| C  | -0.706428152 | 8.147682219  | 6.195140426  |
| C  | -1.111353272 | 8.327593275  | 8.595684466  |
| C  | 0.475544966  | 9.855024829  | 7.507490545  |
| C  | -0.872986202 | 8.961365642  | 9.818544735  |
| C  | -0.046796143 | 8.585037231  | 5.026704257  |
| C  | -1.616623910 | 7.067647351  | 6.127176522  |
| C  | 0.711760134  | 10.480085365 | 8.762512692  |
| C  | 1.659972248  | 11.609919364 | 8.907707418  |
| C  | 0.014833009  | 10.032632710 | 9.894284181  |
| C  | -2.007263804 | 7.251009003  | 8.516342426  |
| C  | 1.150151235  | 10.246437362 | 6.329429127  |
| C  | -2.257275306 | 6.625630259  | 7.292506070  |
| C  | 0.881826473  | 9.627355529  | 5.106812570  |
| C  | -0.313316000 | 7.956347904  | 3.801468400  |
| C  | -1.864370411 | 6.446040673  | 4.894283378  |
| C  | -1.217963237 | 6.893128088  | 3.738795274  |
| C  | 7.449180269  | 12.608674029 | 13.334305893 |
| C  | 6.322990442  | 12.457514395 | 12.529184954 |
| C  | 5.367996049  | 11.480635559 | 12.790097828 |
| C  | 5.503536761  | 10.617871696 | 13.876414279 |
| C  | 6.633813778  | 10.753868543 | 14.700926539 |
| C  | 7.601755831  | 11.743464329 | 14.430799881 |
| S  | 5.869367771  | 13.364180215 | 11.151413350 |
| C  | 4.445648283  | 12.444972503 | 10.952525325 |
| N  | 4.331851348  | 11.474180707 | 11.906324178 |
| Cu | 2.627827363  | 10.576517273 | 11.545076009 |
| H  | 1.407465514  | 7.354719202  | 13.003063563 |
| H  | 5.561597108  | 10.233392099 | 8.100193206  |
| H  | 2.481185355  | 6.660640863  | 10.958203600 |
| H  | 4.624252690  | 9.543305122  | 10.244297668 |
| H  | 5.718819493  | 9.975722416  | 5.657535519  |

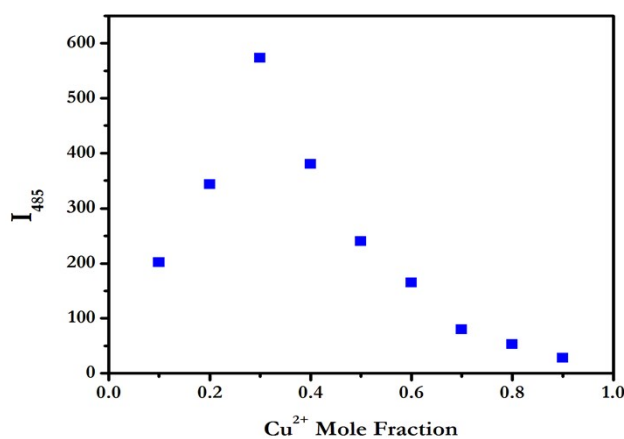
|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 1.411142874  | 6.056564814  | 9.143334189  |
| H | 5.059154177  | 8.830447710  | 3.592050103  |
| H | 0.813096587  | 4.913671046  | 7.099572015  |
| H | 1.059951794  | 4.592660878  | 4.666196059  |
| H | 3.726688185  | 7.099534750  | 2.433907083  |
| H | 2.074378678  | 5.270329359  | 2.523041260  |
| H | -1.346222088 | 11.341857655 | 16.530954607 |
| H | 1.474574896  | 13.427862336 | 12.958325353 |
| H | 0.206581175  | 14.866241775 | 14.561841976 |
| H | -1.197024385 | 13.830363679 | 16.336368162 |
| H | 3.630627341  | 13.339499297 | 9.231790399  |
| H | -1.385728374 | 8.636692971  | 10.720159330 |
| H | 1.767595600  | 12.321489049 | 8.091486356  |
| H | 0.139980279  | 10.535180107 | 10.843797399 |
| H | -2.519040099 | 6.892370044  | 9.405454563  |
| H | 1.904390434  | 11.023367650 | 6.333533676  |
| H | -2.956146271 | 5.794244352  | 7.257099538  |
| H | 1.417703099  | 9.956314725  | 4.220320429  |
| H | 0.188749631  | 8.278453884  | 2.893174370  |
| H | -2.558675973 | 5.613149520  | 4.823885660  |
| H | -1.412793643 | 6.406002548  | 2.788598057  |
| H | 8.187875089  | 13.375182381 | 13.122705657 |
| H | 4.755375107  | 9.857809363  | 14.080518767 |
| H | 6.762343824  | 10.092519726 | 15.551919044 |
| H | 8.469671993  | 11.839015764 | 15.075436031 |



**Fig. S16** ESI-MS of **TyM** with  $\text{Cu}^{2+}$ .

#### **Jobs Plot Analysis of **TyM** with $\text{Cu}^{2+}$ :**

In order to assess the stoichiometric ratio of the chemoreceptor **TyM** with  $\text{Cu}^{2+}$  successive solutions comprising of  $5 \times 10^{-5}$  M  $\text{Cu}(\text{SO}_4)_2$  and **TyM** were prepared in acetonitrile solvent in such a way that the total concentration of the resulting solution remains constant. The mole fraction of the added analyte  $\text{Cu}^{2+}$  was varied from 0.1 to 0.9. The emission of the chemoreceptor **TyM** at 485 nm has been plotted against the mole fraction of the added analyte. From the Jobs Plot analysis it clearly affirms a 2:1 complexation between the host chemoreceptor **TyM** and the guest analyte (Fig. S17).



**Fig. S17** Job's plot of chemoreceptor **TyM** with  $\text{Cu}^{2+}$  with a total concentration of  $5 \times 10^{-5}$  M.

#### **Cell culture, imaging details:**

The bio-imaging system consisted of an inverted fluorescence microscope (Leica DM 1000 LED), digital compact camera (Leica DFC 420C), and an image processor (Leica Application Suite v3.3.0). The microscope was equipped with a mercury 50 Watt lamp.

### Preparation of *Monilia Albicans* (prokaryotic cell, diploid fungus) and male microspores of seed plants (*Bohonia Nigalandra*) for intracellular detection of Cu<sup>2+</sup>:

Two different types of cells viz. *Monilia Albicans* (prokaryotic cell, diploid fungus) and male microspores of seed plants (*Bohonia Nigalandra*). *Monilia Albicans* cells that have been obtained from exponentially growing culture in the yeast extract glucose broth medium (pH 6.0 and an incubation temperature of 37°C) were washed by suspending them in normal saline and centrifuged at 3000 rpm for approximately 10 minutes. It was then washed thrice with 0.1 M HEPES buffer (pH 7.4). Then the cells were incubated in 50nM Cu<sup>2+</sup> for 45 minutes. After incubation, the cells were thoroughly washed with HEPES buffer and then again incubated with the developed chemoreceptor **TyM** (10 μM) for another span of 1 hour. The treated cells of the developed chemoreceptor **TyM** were again washed by centrifugation (3000 rpm for 5 minutes) using HEPES buffer. Finally the cells procured in this way were mounted on grease free glass slide and thereby observed under a Leica DM 1000 Fluorescence microscope with UV filter to obtain the bright cyan emission which affirms the intracellular imaging of Cu<sup>2+</sup> in the presence of the chemoreceptor **TyM**.

**Detection limit (DL) has been calculated through the following equation<sup>3</sup>:**

$$DL = CL \times ET$$

CL = Conc. of Chemoreceptor **TyM**; ET = Conc. of titrant at which change is observed.

| Detection limit for Cu <sup>2+</sup>                               | Detection limit for CN <sup>-</sup>                               |
|--|---|
| DL = $1 \times 10^{-5} \times 0.004$ equiv = $4 \times 10^{-8}$ M. | DL = $1 \times 10^{-5} \times 0.003$ equiv = $3 \times 10^{-8}$ M |

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